MATHEMATICAL REPRESENTATION OF ISOTOPIC GAS MIGRATION FROM AN UNDERGROUND NUCLEAR WEAPON TEST THROUGH ROCK

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ABSTRACT

An isotopic spectrum from localized air samples has potential technical information to provide a rapid first-order yield estimate of an underground nuclear explosion (UNE) or a simple yes/no detection of a UNE in the context of On-site Inspection (OSI). The isotopic spectrum is presumed to be derived from environmental air samples near the location of the UNE containing nuclear products from the fission reaction of the explosion. Additionally, a seismic spectrum is derived from the sensed ground motion caused by the coupled energy of the UNE to the earth. A mathematical representation of these two measurements has two essential terms in common—the origin time of the event t_0 and the log yield $W = \log_{10} Y$ of the explosion (kilotons TNT). A critical component of the mathematical framework for yield estimation from nuclear measurements is the mathematical representation of isotopic gas migration through rock to the air. This research will complete the scientific development leading to a mathematical representation of isotopic gas migration through rock, and validate the mathematics through simulation studies. If successful, this research has the potential to fully enable a rapid, first-order estimate of the yield of a UNE, or UNE yes/no detection in many monitoring settings.

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OBJECTIVES

If this project is successful, it will offer an analytical expression of gas diffusion through fractured rock, with sufficient accuracy for field use. Additionally, this project will develop a statistical framework for yield estimation that rigorously, smoothly transitions from low-count spectra to high-count Poisson statistics. This framework will be generally applicable and easily improved as research on the components in Equation 1 is improved. For this project, we focus on a current bottleneck to developing a simple first-order solution to yield estimation—gas diffusion through fractured rock.

In the context of UNE, let the counts in a detector energy bin from isotopic gas G be the counting process $N(t)$ with expectation (mean)

$$E\{N(t) \mid \mu\} = \mu\,\eta/\omega\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}\,P_R(t_1-t_0)\,P_C(t_2-t_1)\,P_S(t_3-t_2)\,P_N(t-t_3)\,P_B\,E \quad, \tag{1}$$

where μ is fissionable mass [= grams], t is the time since event origin t_0, and $T_{1/2}$ is the half-life of the isotopic gas G. From left to right, ω is the atomic weight [= grams/mole], η is Avogadro's number [= atom/mole] and so $N_0=\mu\,\eta/\omega$ is the number of atoms available for fission. $N_0\,P_F$ are the atoms that fission. UNE yield Y is reported in kilotons of TNT and to first order $Y=\kappa\,N_0\,P_F$, where κ scales energy release from fissions to equivalent chemical energy release. $N_0\,P_F\,P_G$ is the number of atoms of a specific isotopic gas produced by the fission atoms. $N_0\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}$ are the number of isotopic gas atoms surviving at time t_1, and $N_0'=N_0\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}\,P_R(t_1-t_0)$ are the number of surviving isotopic gas atoms that migrate through rock into the air and are available for collection t_1-t_0 after the event. This migration is represented by the factor $P_R(t_1-t_0)$ and the fundamental objective of this research effort is the development of an analytical mathematical representation of $P_R(t_1-t_0)$ or potentially a single mathematical representation for N_0'.

Make the assumption that the environmental sampling process has a constant collection rate and that the isotopic gas G is homogeneously mixed and that the mixing composition is constant throughout collection. $N_0\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}\,P_R(t_1-t_0)\,P_C(t_2-t_1)$ are the isotopic gas atoms acquired from collection by time t_2. $N_0\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}\,P_R(t_1-t_0)\,P_C(t_2-t_1)\,P_S(t_3-t_2)$ are the atoms available for the gamma-ray spectrum after separations. Finally, $N_0\,P_F\,P_G\,exp\{-(t_1-t_0)\,ln(2)/T_{1/2}\}\,P_R(t_1-t_0)\,P_C(t_2-t_1)\,P_S(t_3-t_2)\,P_N(t-t_3)$ are the gas atoms that decay in the nuclear counting process, and to complete the equation P_B is the absolute branching probability of the gas isotope for the energy associated to the detector bin (energy bin), and E is the detector efficiency. Appropriate for this project, the factors $P_C(t_2-t_1), P_S(t_3-t_2)$, and $P_N(t-t_3)$ are analytically derived with probability calculations in Anderson et al. (2007). Specifically, with the probability an atom decays in time Δt given by $\lambda\,\Delta t$,

$$P_C(t_2-t_1) = (1-exp\{-\lambda\,(t_2-t_1)\})/(\lambda\,(t_2-t_1)), \tag{2}$$

$$P_S(t_3-t_2) = exp\{-\lambda\,(t_3-t_2)\} \text{ and} \tag{3}$$

$$P_N(t-t_3) = 1-exp\{-\lambda\,(t-t_3)\}. \tag{4}$$

Equation (1) provides model components to represent the probabilistic relationship between the number of radioactive atoms in an acquired gas sample and observed radioactive detector counts. Nuclear disintegration for a specific spectral energy bin is modeled as a Poisson processes, that is, the random variable $N(t) \mid \mu$ is Poisson with mean $E\{N(t) \mid \mu\}$. This probability model is the foundation for the development of a diverse suite of algorithms relevant to treaty verification and nuclear explosion monitoring.

The Los Alamos National Laboratory (LANL) soil vapor extraction (SVE) model builds on the Los Alamos porous flow simulator, the Finite Element Heat and Mass (FEHM) transfer code, a one-, two-, and three-dimensional finite-volume heat and mass transfer code (Zyvoloski et al., 2008). This model has been used extensively for simulation of multiphase transport and has wide capabilities to simulate subsurface flow and transport systems with complicated geometries in multiple dimensions (Stauffer et al., 1997, 2005; Stauffer and Rosenberg, 2000; Neeper and Stauffer, 2005; Kwicklis et al., 2006; and many others). Equations governing the conservation of phase mass, contaminant moles, and energy are solved numerically using a fully implicit Newton–Raphson scheme. Capabilities have been

added as needed through the years, and LANL now maintains one of the most robust porous media gas transport codes available anywhere in the world. A recent code modification allows CO_2 to be simulated across the critical point in high pressure and temperature systems (Stauffer et al., 2009a). Another exciting new development is the addition of parameter estimate software that allows parameter space to be explored efficiently (e.g., Stauffer et al., 2009b). The reactive chemistry section of the code is highly versatile, with species in both the liquid and vapor able to react with rock to form and dissolve minerals Chaudhuri, et al., 2009).

FEHM has been expanded to include the equations for stress and strain which allow us to model rock fracture induced by increasing fluid pressures (Deng et al., 2009). Current work on hydrofracture induced by the injection of CO_2 can readily be adapted to the work proposed here on subsurface gas migration through explosively generated fractures toward the atmosphere. As confining stress in the model is decreased, fractures are opened in the plane perpendicular to the minimum principle stress, and permeability functions are updated.

Project Plan

There are three core tasks for this project, which stop short of validating the developed mathematics with observational data from the Nevada National Security Site (NNSS). Potential follow-on validation studies could conceivably begin as early as the summer of 2013It is conceivable that the validation studies could begin as early as the summer of 2013 should the appropriate experimental data be available from activities at NNSS (see Brunish et al.; Mellors et al.; Antoun et al; and Snelson et al., these Proceedings).

Task 1 (Year 1): Perform FEHM Simulations of Gas Diffusion through Fractured Rock

Task 1 of the project will configure and parametrize the LANL FEHM code to simulate gas diffusion through fractured rock. Parametrization of the code will span a suite of rock composition and fracturing. Simulation output will be captured as the proportion of gas that escapes to the surface as a function of depth and the suite of rock composition and fracturing configurations. Reasonable assumptions will be necessary to complete this task—these will be researched and mathematically identified. Code configurations will be validated with data acquired from NNSS experiments.

Task 2 (Year 2): Develop Analytical (Statistical) Representation of Gas Diffusion Simulation Output

Task 2 of the project will research and/or develop an analytical probability model of gas diffusion through fractured rock. Assumptions will be necessary to complete this derivation. This analytical statistical model will be compared to the simulation output in Task 1 and adapted/enhanced to achieve acceptable agreement with simulated data. Several metrics of agreement will be identified and used in this effort. The final analytical model from this task will move forward to the development of confidence interval equations/algorithms for explosion yield and identification.

Task 3 (Year 3): Develop Ensemble Analytical Model (Physical and Statistical) Linking Explosion Mass to Observed Spectrum and Derive Confidence Interval Equations/Algorithms for Explosion Yield

The goal of Task 3 is the development of analytical equations/algorithms for a confidence interval of an explosion yield. The Bayesian approach to yield estimation in Anderson et al. (2006), for low-count spectra, will be leveraged into this development. Here, a non-informative prior distribution is placed on radioactive mass, ensuring that the estimate of mass is always positive and the estimation equation is the same as that derived with high-count Poisson statistics. This Bayesian approach will provide relevant methods for the concept of operations that this research can enable.

RESEARCH ACCOMPLISHED

Project was initiated in June 2011.

CONCLUSIONS

The project will execute fundamental research to enable timely yield estimation of an underground nuclear explosion using a near-to source observed isotopic gas spectrum.

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